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Weakly frustrated spin-$\frac{1}{2}$ Heisenberg antiferromagnet in two dimensions: Thermodynamic parameters and the stability of the Néel state

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Using a Schwinger-boson mean-field theory, we calculate the low-temperature uniform transverse susceptibility $\chi_\perp$ and spin-wave velocity c for the weakly frustrated spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet with exchange couplings J_1, J_2, and J_3 to first, second, and third neighbors. By connecting $\chi_\perp$ and c to the bare coupling of the nonlinear σ model that describes the long-wavelength limit of the antiferromagnet, we are able to improve upon earlier renormalization-group estimates of the zero-temperature phase boundary separating Néel and magnetically disordered ground states. To one-loop level in an ϵ expansion we find a disordering transition across a line joining the points $(J_2,J_3)/J_1=(0.15,0)$ and $(0,0.09)$. Thus, the classical phase boundary $(J_2+2J_3)/J_1=\frac{1}{2}$ is shifted asymmetrically by quantum fluctuations, as expected when the transition is to a columnar dimerized ground state.

Introduction. As seen in recent developments, the discovery of two-dimensional (2D) magnetic structures in the high-T_c superconductors has sparked an intense interest in low-dimensional antiferromagnets.[1] In particular, much effort has been invested in understanding the effects of the zero-temperature quantum fluctuations on the 2D ground state for spin $S=\frac{1}{2}$. Contrary to early suggestions, there is now strong evidence that the $T=0$ ground state of the spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet with nearest-neighbor exchange is *not* disordered by quantum fluctuations.[2] However, things turn more controversial when adding exchange interactions between next-nearest neighbors. This gives the J_1-J_2 model

$$\mathcal{H}_{12}=J_1\sum_{\mathbf{R},\boldsymbol{\alpha}}\mathbf{S}_\mathbf{R}\cdot\mathbf{S}_{\mathbf{R}+\boldsymbol{\alpha}}+J_2\sum_{\mathbf{R},\boldsymbol{\beta}}\mathbf{S}_\mathbf{R}\cdot\mathbf{S}_{\mathbf{R}+\boldsymbol{\beta}}, \qquad (1)$$

with $J_1,J_2\geq 0$, and where the sums run over all lattice sites $\mathbf{R}$ with attached spin operators $\mathbf{S}_\mathbf{R}$, as well as over $\boldsymbol{\alpha}$ $(=\mathbf{e}_x,\mathbf{e}_y)$ and $\boldsymbol{\beta}$ $(=\mathbf{e}_x\pm\mathbf{e}_y)$, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ denoting lattice vectors to half the number of nearest and next-nearest neighbors, respectively. Studies exploiting modified spin-wave theories[3] and their equivalents[4] (as well as the physical $N=1$ limit of certain $1/N$ expansions[5]) predict a first-order transition at $J_2/J_1\approx 0.6$, separating the semiclassically established Néel and collinear states. In contrast, series expansions,[6] self-consistent perturbations,[7] numerical studies,[8] and certain mean-field constructions[9] suggest that a spontaneously dimerized (spin-Peierls) phase may open up for some intermediate range of values of the frustrating coupling J_2. Other proposals for magnetically disordered phases have also been made, such as the chiral and twisted spins liquids.[1]

Some time ago, two of us[10] used a renormalization-group (RG) approach to address the problem of Néel stability for an extension of the Hamiltonian in (1), the J_1-J_2-J_3 model:

$$\mathcal{H}_{123}=\mathcal{H}_{12}+J_3\sum_{\mathbf{R},\boldsymbol{\alpha}}\mathbf{S}_\mathbf{R}\cdot\mathbf{S}_{\mathbf{R}+2\boldsymbol{\alpha}}, \qquad (2)$$

with $J_3\geq 0$. For large spin, and in the presence of local Néel order (*weak frustration*), the dynamics of the order parameter was found to be governed by a quantum nonlinear σ model with a bare coupling g_0 given by

$$g_0=\frac{S}{\sqrt{S(S+1)}}\frac{1}{c\chi_\perp}. \qquad (3)$$

Here c, the spin-wave velocity, and $\chi_\perp$, the uniform transverse susceptibility, are given by the same expressions as in spin-wave theory (SWT), using units where $g\mu=1$.[11] With $\alpha\equiv(J_2+2J_3)/J_1$, one has $c=\sqrt{8(1-2\alpha)}J_1S$ and $\chi_\perp=1/(8J_1)$, the latter being independent of frustration. From a one-loop recursion relation for the infrared coupling flow of the model,[12] and a physically proper lattice regularization,[10] a zero-temperature disordering transition at the fixed point value $g_0=4\sqrt{\pi}$ was obtained. This then gives a critical frustration α_c. For *any* spin $S\geq\frac{1}{2}$, the result closely mimics that obtained by studying $O(1/S)$ corrections to the sublattice magnetization in SWT,[13] supporting the use of a one-loop approximation for the fixed point.[14]

Turning to small spins, the semiclassical parameters in (3) will pick up corrections from quantum fluctuations. We argued in Ref. 10 that these corrections can depend only weakly on the frustrating couplings J_2 and J_3, so that we could use the quantum corrections for the unfrustrated interaction to a good approximation. For spin $\frac{1}{2}$, the correction factors are $Z_c=1.18\pm 0.02$ and $Z_{\chi_\perp}=0.52\pm 0.03$.[15,16] Inserting these numbers into (3) one finds a transition at $\alpha_c=0.22\pm 0.04$. This is substantially lower than the semiclassical prediction $\alpha_c\approx 0.4$, as expected in the presence of strong destabilizing quantum fluctuations. However, considering the very large discrepancy between this result and that of the modified spin-wave theories,[3,4] where the Néel state is actually stabilized beyond the classical boundary ($\alpha_c\approx 0.6$), the issue needs to be reexamined. This we shall do in the present paper by attempting a direct calculation of c and $\chi_\perp$ in the *presence of frustra-*

tion. Rather strikingly, our improved stability estimate reveals a signature characteristic of a transition to a columnar dimerized phase.

Schwinger-boson mean-field theory (SBMFT). Inspired by the success of the SBMFT to cleanly produce the parameters c and $\chi_\perp$ for the unfrustrated spin-$\frac{1}{2}$ Heisenberg model,[16] this is the method we choose also for the present problem. Since the SBMFT yields good estimates of these parameters in the presence of disordering thermal fluctuations, we do expect the theory to be applicable also in the presence of enhanced quantum fluctuations due to (weak) frustration.

Following Arovas and Auerbach,[16] we introduce two boson operators $b_{\mu\mathbf{R}}^\dagger$ ($\mu=1,2$), and write

$$\mathbf{S}_\mathbf{R}=\tfrac{1}{2}\,b_{\mu\mathbf{R}}^\dagger\sigma_{\mu\nu}b_{\nu\mathbf{R}}\,, \tag{4}$$

with the local constraints $b_{\mu\mathbf{R}}^\dagger b_{\mu\mathbf{R}}=2S$. Here $\boldsymbol{\sigma}=(\sigma^x,\sigma^y,\sigma^z)$ are the Pauli matrices, and summation over repeated (Greek) indices is implied. By a π rotation of the spin operators (and the corresponding local states) around the y axis on one sublattice, the Hamiltonian in (2) gets transformed into

$$\mathcal{H}_{123}=-J_1\sum_{\mathbf{R},\alpha}\mathcal{W}^{\mathcal{A}}_{\mathbf{R},\alpha}+J_2\sum_{\mathbf{R},\beta}\mathcal{W}^{\mathcal{B}}_{\mathbf{R},\beta}+J_3\sum_{\mathbf{R},\alpha}\mathcal{W}^{\mathcal{B}}_{\mathbf{R},2\alpha}+\sum_{\mathbf{R}}\lambda_\mathbf{R}[b_{\mu\mathbf{R}}^\dagger b_{\mu\mathbf{R}}-2S]\,, \tag{5}$$

where the last term has been added to enforce the local constraints, and the summands are defined through

$$\mathcal{W}^{\mathcal{X}}_{\mathbf{R},\boldsymbol{\delta}}=\tfrac{1}{2}:\mathcal{X}^\dagger_{\mathbf{R},\boldsymbol{\delta}}\mathcal{X}_{\mathbf{R},\boldsymbol{\delta}}:-S^2\,. \tag{6}$$

The link operators remain to be defined:

$$\mathcal{A}_{\mathbf{R},\boldsymbol{\delta}}\equiv b_{1\mathbf{R}}b_{1\mathbf{R}+\boldsymbol{\delta}}+b_{2\mathbf{R}}b_{2\mathbf{R}+\boldsymbol{\delta}}\,, \tag{7a}$$

$$\mathcal{B}_{\mathbf{R},\boldsymbol{\delta}}\equiv b_{1\mathbf{R}}^\dagger b_{1\mathbf{R}+\boldsymbol{\delta}}+b_{2\mathbf{R}}^\dagger b_{2\mathbf{R}+\boldsymbol{\delta}}\,. \tag{7b}$$

To generate a mean-field theory, we do the Hartree-Fock decoupling

$$:\mathcal{X}^\dagger_{\mathbf{R}\boldsymbol{\delta}}\mathcal{X}_{\mathbf{R}\boldsymbol{\delta}}:\rightarrow\mathcal{X}^\dagger_{\mathbf{R}\boldsymbol{\delta}}\langle\mathcal{X}_{\mathbf{R}\boldsymbol{\delta}}\rangle+\langle\mathcal{X}^\dagger_{\mathbf{R}\boldsymbol{\delta}}\rangle\mathcal{X}_{\mathbf{R}\boldsymbol{\delta}}-\langle\mathcal{X}^\dagger_{\mathbf{R}\boldsymbol{\delta}}\rangle\langle\mathcal{X}_{\mathbf{R}\boldsymbol{\delta}}\rangle\,, \tag{8}$$

and assume that the condensates $Q_1\equiv\langle\mathcal{A}_{\mathbf{R},\alpha}\rangle$, $Q_2\equiv\langle\mathcal{B}_{\mathbf{R},\beta}\rangle$, and $Q_3\equiv\langle\mathcal{B}_{\mathbf{R},2\alpha}\rangle$ are uniform and real. As long as the frustration is weak and does not change the character of the ground state, this assumption is reasonable since real condensates have been shown to minimize the free energy of the unfrustrated model.[16]

Replacing the local Lagrange multiplier $\lambda_\mathbf{R}$ by a single parameter λ, the resulting mean-field Hamiltonian is easily diagonalized in momentum space, and yields free bosons with dispersion relation

$$\omega_\mathbf{k}=[(\lambda+2J_2Q_2\gamma_{2,\mathbf{k}}+2J_3Q_3\gamma_{3,\mathbf{k}})^2-(2J_1Q_1\gamma_{1,\mathbf{k}})^2]^{1/2}\,. \tag{9}$$

The geometrical factors are here given by

$$\gamma_{1,\mathbf{k}}=\gamma_{3,(1/2)\mathbf{k}}=\tfrac{1}{2}(\cos k_x+\cos k_y)\,, \tag{10a}$$

$$\gamma_{2,\mathbf{k}}=\cos k_x\cos k_y\,. \tag{10b}$$

For any set of fixed values of J_1, J_2, J_3, and inverse temperature $\beta=1/k_BT$, the parameters λ, Q_1, Q_2, and Q_3 are obtained by numerically solving the integral equations corresponding to a stationary free energy:

$$\int\frac{d^2k}{(2\pi)^2}\cosh(2\theta_\mathbf{k})(n_\mathbf{k}+\tfrac{1}{2})-(S+\tfrac{1}{2})=0\,, \tag{11a}$$

$$\int\frac{d^2k}{(2\pi)^2}\sinh(2\theta_\mathbf{k})\gamma_{1,\mathbf{k}}(n_\mathbf{k}+\tfrac{1}{2})-\tfrac{1}{2}Q_1=0\,, \tag{11b}$$

$$\int\frac{d^2k}{(2\pi)^2}\cosh(2\theta_\mathbf{k})\gamma_{j,\mathbf{k}}(n_\mathbf{k}+\tfrac{1}{2})-\tfrac{1}{2}Q_j=0\,, \tag{11c}$$

with $j=2,3$. Here $n_\mathbf{k}=[\exp(\beta\omega_\mathbf{k})-1]^{-1}$ is the Bose distribution function, and $\theta_\mathbf{k}$ is given by

$$\tanh(2\theta_\mathbf{k})=\frac{2J_1Q_1\gamma_{1,\mathbf{k}}}{\lambda+2J_2Q_2\gamma_{2,\mathbf{k}}+2J_3Q_3\gamma_{3,\mathbf{k}}}\,. \tag{12}$$

Turning off J_2 and J_3, these equations collapse to those obtained by Arovas and Auerbach[16] for the ordinary Heisenberg model via a functional-integral method. In our case, however, the frustrating terms in (5) come with the "wrong sign," and preclude a similar treatment.

Thermodynamic parameters. The spin-wave velocity c, as well as the mass m, of the excitations, can be obtained by expanding (9) to second order in $\mathbf{k}$ and writing $\omega_\mathbf{k}$ in the form $\omega_\mathbf{k}=c[(mc)^2+\mathbf{k}^2]^{1/2}$. This yields

$$c=[2J_1^2Q_1^2-2(J_2Q_2+2J_3Q_3)(\lambda+2J_2Q_2+2J_3Q_3)]^{1/2}\,, \tag{13}$$

$$mc^2=[(\lambda+2J_2Q_2+2J_3Q_3)^2-(2J_1Q_1)^2]^{1/2}\,. \tag{14}$$

The mass m goes to zero as $T\rightarrow0$, since the excitation spectrum is gapless in the Néel state.

To obtain the spin-wave velocity c in the $T\rightarrow0$ limit, we have solved Eqs. (11) for $S=\frac{1}{2}$ in the temperature range $3<J_1\beta<11$, fitted c to a power series in T, and extrapolated down to $T=0$. As a check, we have also calculated c *at* $T=0$ by using a zero-temperature version of SBMFT. The resulting c is plotted versus the frustrating coupling in Fig. 1. The three slices of coupling space that we have chosen are $(J_2,J_3)/J_1=(0,\alpha/2)$, $(\alpha/2,\alpha/4)$, and $(\alpha,0)$, with $0\le\alpha\le\frac{1}{2}$ ($\alpha=\frac{1}{2}$ being the classical transition point).

In the unfrustrated case, the mass $m\propto\exp(-\text{const}/T)$ as $T\rightarrow0$.[1] Since frustration increases the magnitude of *quantum fluctuations*, whereas temperature increases *thermal fluctuations*, it is interesting to examine how the mass varies with frustration at a fixed finite temperature. Even if we have not made any extensive analysis, it appears that m scales with frustration as an exponential for small α, as indicated in Fig. 2.

Turning to the uniform susceptibility, its rotational average $\bar{\chi}$ is connected to the structure factor $\mathcal{S}_{xx}(\mathbf{q},t)$ by

$$\bar{\chi}=\frac{1}{k_BT}\mathcal{S}_{xx}(\mathbf{q}=0,t=0)\,, \tag{15}$$

where

$$\mathcal{S}_{xx}(\mathbf{q}=0,t=0)=\frac{2}{3}\int\frac{d^2k}{(2\pi)^2}\,\tfrac{1}{2}\,n_\mathbf{k}(n_\mathbf{k}+1)\,. \tag{16}$$

Here, a factor $\frac{2}{3}$ has been inserted in the right-hand side

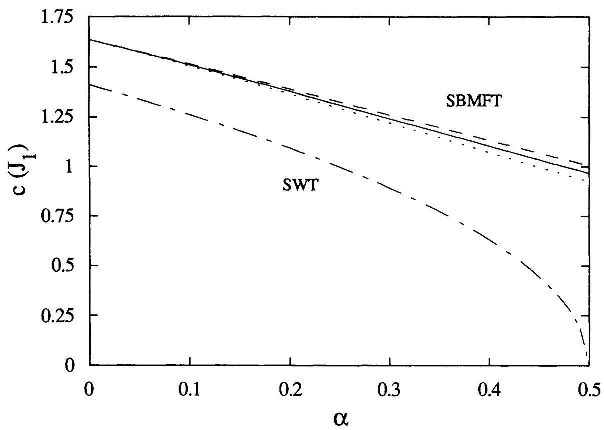

FIG. 1. The $T=0$ spin-wave velocity vs frustration α. The lines correspond to (from the top) SBMFT with $(J_2,J_3)/J_1=(0,\alpha/2)$, $(\alpha/2,\alpha/4)$, and $(\alpha,0)$, and SWT, respectively.

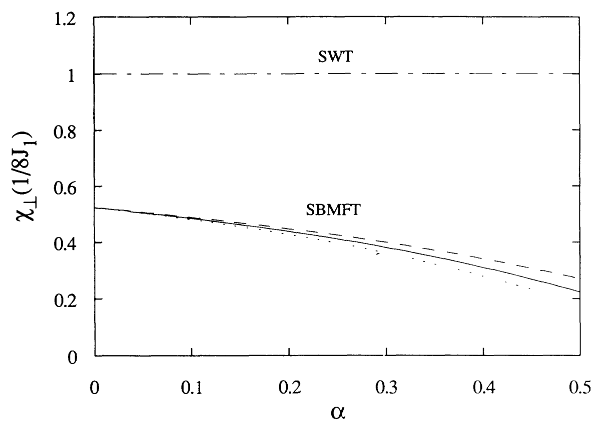

FIG. 3. The $T=0$ uniform transverse susceptibility vs frustration. The lines correspond to SWT and SBMFT with (from the top) $(J_2,J_3)/J_1=(0,\alpha/2)$, $(\alpha/2,\alpha/4)$, and $(\alpha,0)$, respectively.

of (16) to correct for the mean-field treatment of the local constraints.[16] At $T=0$ (Néel state), the longitudinal component $\chi_\parallel$ should vanish, and hence the transverse component $\chi_\perp=\frac{3}{2}\bar{\chi}$. In Fig. 3 we have plotted the $T=0$ extrapolations of $\chi_\perp$ for the same slices of coupling space as above. As seen in Figs. 1–3, all three parameters, c, m, and $\chi_\perp$, exhibit a weak anisotropy in coupling space, with the anisotropy increasing with the magnitude of the frustration α. Let us stress that the region where we expect our SBMFT results to be reliable is roughly constrained by the Néel boundary, to be estimated next.

Stability of the Néel state. We now use the SBMFT values for $\chi_\perp$ and c to improve upon the estimate of the phase boundary of the Néel state. To do this we use Eq. (3) with the SWT parameters replaced by the SBMFT parameters, and with g_0 at the fixed point $4\sqrt{\pi}$.[10] The phase boundary is thus given by the solutions in $(J_2,J_3)/J_1$ space to the equation

$$\frac{1}{c\chi_\perp}=4\sqrt{3\pi}\,. \quad (17)$$

The phase diagram we arrive at is shown in Fig. 4. The new Néel boundary is almost a straight line, joining the points $J_2/J_1=0.154\pm0.004$ and $J_3/J_1=0.089\pm0.002$. (The estimated uncertainty is entirely due to our numerical calculations.) The classical boundary $\alpha_c=\frac{1}{2}$ is seen to be shifted more by quantum fluctuations along the J_2 axis than along J_3. This phenomenon has been observed earlier in the transition from a columnar dimerized state to a Néel state.[6,9] The reason appears to be that the J_2 coupling stabilizes the columnar phase more than J_3 does, because it acts directly in competition with J_1 in the matrix element of "resonance" of nearest-neighbor parallel dimers.[17] It is important to stress that our calculation, in contrast to Refs. 6 and 9, detects this asymmetric shift via a method that does *not favor the formation of a columnar phase.* While our boundary points $(J_2,J_3)/J_1=(0.15,0)$ and $(0,0.09)$ are lower than those in Ref. 6, they are close to the result in Ref. 9 where $(J_2,J_3)/J_1=(0.19,0)$ and $(0,0.13)$.

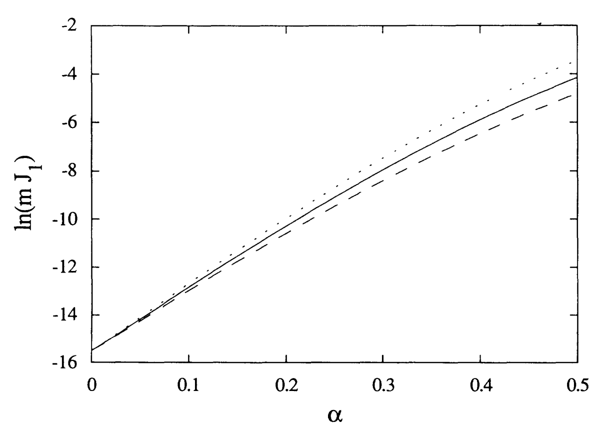

FIG. 2. The logarithm of the mass vs frustration for SBMFT at temperature $\beta=11/J_1$. The curves correspond to (from the bottom) $(J_2,J_3)/J_1=(0,\alpha/2)$, $(\alpha/2,\alpha/4)$, and $(\alpha,0)$, respectively.

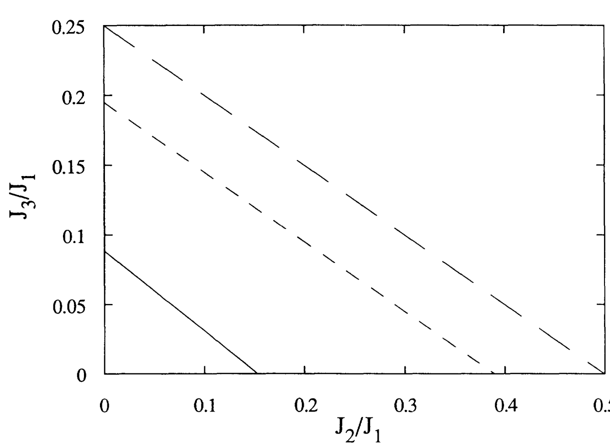

FIG. 4. The $T=0$ phase diagram for the J_1-J_2-J_3 model with $S=\frac{1}{2}$. The solid line marks the Néel boundary obtained in this paper, while the short-dashed line shows the semiclassical σ model result, with SWT values for c and $\chi_\perp$. The long-dashed line represents the classical result.

Summary. To the extent that SBMFT is a reliable guide to estimate the parameters c and $\chi_\perp$ for weak frustration, our result indicates, to one-loop level in an ϵ expansion, that the domain of Néel stability for the spin-$\frac{1}{2}$ J_1-J_2-J_3 model is strongly reduced by quantum fluctuations. The asymmetric shift of the classical phase boundary further suggests a transition to a columnar dimerized ground state.

It remains to be explained why the zero-temperature version of the SBMFT, as exploited by Mila and coworkers,[4] yields a result in conflict with ours. These authors find a transition for the J_1-J_2 model at $J_2/J_1 \approx 0.6$, to be compared with our prediction $J_2/J_1 = 0.15$. The Néel domain in Ref. 4 is identified by looking for solutions of the $T=0$ analogs of our mean-field equations in (11) (with $J_3=0$) in the presence of a Bose condensate. In other words, the mean-field theory is used to directly probe the order parameter, which sensitively depends on fluctuations. Also, it is *assumed* that there are no intermediate phases in between the regions of Néel and collinear order. In contrast, in our approach *no* assumption is made about the character of the state on the other side of the boundary. Further, we use the SBMFT to probe quantities which do not change character across the transition, and hence are less sensitive to fluctuations. The phase boundary is instead located by a renormalization-group argument, with the mean-field values of these parameters as input data. From our experience with classical phase transitions, it seems that the latter approach should be the more reliable. However, more work is needed to conclusively resolve the issue.

Note added in proof. Yoshioka has informed us that a SBMFT calculation of the susceptibility at $T=0$ in the presence of a magnetic field may yield slightly larger values of $\chi_\perp$ than reported here (where possible vertex corrections due to the magnetic field have been neglected). This would imply a somewhat larger Néel phase than shown in Fig. 4. See D. Yoshioka, J. Phys. Soc. Jpn. **58**, 3733 (1989).

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